

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092622\  
 Data File : VU050937.D  
 Acq On : 26 Sep 2022 10:55  
 Operator : JC/MD  
 Sample : VU0926WBL01  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 VBLK187

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M

Title : VOC Analysis

Signal : TIC: VU050937.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.601       | 73            | 81          | 97           | rVB      | 239347         | 279581        | 14.51%          | 1.983%        |
| 2         | 1.913       | 169           | 178         | 193          | rBV      | 202558         | 261825        | 13.58%          | 1.857%        |
| 3         | 2.568       | 368           | 382         | 400          | rBV      | 387827         | 637034        | 33.05%          | 4.519%        |
| 4         | 2.761       | 440           | 442         | 444          | rBV      | 459            | 275           | 0.01%           | 0.002%        |
| 5         | 2.790       | 446           | 451         | 461          | rVB3     | 1584           | 2781          | 0.14%           | 0.020%        |
| 6         | 2.951       | 496           | 501         | 503          | rVV3     | 419            | 419           | 0.02%           | 0.003%        |
| 7         | 3.044       | 524           | 530         | 539          | rVB4     | 3137           | 4469          | 0.23%           | 0.032%        |
| 8         | 3.186       | 564           | 574         | 584          | rBV3     | 1508           | 3191          | 0.17%           | 0.023%        |
| 9         | 3.302       | 607           | 610         | 613          | rBV2     | 327            | 258           | 0.01%           | 0.002%        |
| 10        | 3.350       | 621           | 625         | 627          | rBV3     | 938            | 682           | 0.04%           | 0.005%        |
| 11        | 3.433       | 642           | 651         | 654          | rBV2     | 373            | 383           | 0.02%           | 0.003%        |
| 12        | 3.498       | 668           | 671         | 676          | rVB2     | 359            | 279           | 0.01%           | 0.002%        |
| 13        | 3.883       | 786           | 791         | 795          | rBV2     | 243            | 289           | 0.01%           | 0.002%        |
| 14        | 3.951       | 807           | 812         | 818          | rBV2     | 233            | 260           | 0.01%           | 0.002%        |
| 15        | 4.086       | 850           | 854         | 858          | rVB      | 271            | 257           | 0.01%           | 0.002%        |
| 16        | 4.321       | 923           | 927         | 931          | rVV2     | 285            | 289           | 0.01%           | 0.002%        |
| 17        | 4.411       | 951           | 955         | 958          | rBV      | 364            | 306           | 0.02%           | 0.002%        |
| 18        | 4.523       | 986           | 990         | 1001         | rBV2     | 365            | 477           | 0.02%           | 0.003%        |
| 19        | 4.620       | 1001          | 1020        | 1058         | rBV      | 216600         | 561613        | 29.14%          | 3.984%        |
| 20        | 5.064       | 1140          | 1158        | 1180         | rBV      | 352867         | 776439        | 40.29%          | 5.508%        |
| 21        | 5.240       | 1210          | 1213        | 1217         | rBV3     | 322            | 261           | 0.01%           | 0.002%        |
| 22        | 5.285       | 1222          | 1227        | 1228         | rBV3     | 756            | 566           | 0.03%           | 0.004%        |
| 23        | 5.334       | 1240          | 1242        | 1244         | rVB3     | 545            | 270           | 0.01%           | 0.002%        |
| 24        | 5.379       | 1252          | 1256        | 1259         | rVV4     | 523            | 410           | 0.02%           | 0.003%        |
| 25        | 5.507       | 1292          | 1296        | 1299         | rBV2     | 315            | 249           | 0.01%           | 0.002%        |
| 26        | 5.726       | 1341          | 1364        | 1394         | rBV2     | 706922         | 1927337       | 100.00%         | 13.673%       |
| 27        | 5.970       | 1437          | 1440        | 1442         | rBV3     | 523            | 282           | 0.01%           | 0.002%        |
| 28        | 6.041       | 1460          | 1462        | 1467         | rVB4     | 667            | 495           | 0.03%           | 0.004%        |
| 29        | 6.247       | 1512          | 1526        | 1555         | rBV      | 490205         | 939093        | 48.72%          | 6.662%        |
| 30        | 6.475       | 1592          | 1597        | 1599         | rBV2     | 339            | 319           | 0.02%           | 0.002%        |
| 31        | 6.530       | 1602          | 1614        | 1630         | rVB3     | 17102          | 33075         | 1.72%           | 0.235%        |
| 32        | 6.690       | 1649          | 1664        | 1694         | rBV      | 459579         | 901674        | 46.78%          | 6.397%        |
| 33        | 7.054       | 1773          | 1777        | 1782         | rVB2     | 430            | 436           | 0.02%           | 0.003%        |
| 34        | 7.192       | 1810          | 1820        | 1824         | rBV3     | 2441           | 3053          | 0.16%           | 0.022%        |
| 35        | 7.353       | 1868          | 1870        | 1879         | rVB2     | 250            | 275           | 0.01%           | 0.002%        |
| 36        | 7.475       | 1900          | 1908        | 1911         | rBV2     | 430            | 434           | 0.02%           | 0.003%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 7.501  | 1911 | 1916 | 1919 | rVB3 | 379    | 305     | 0.02%  | 0.002% |
| 38 | 7.565  | 1923 | 1936 | 1958 | rBV  | 224921 | 403820  | 20.95% | 2.865% |
| 39 | 7.690  | 1970 | 1975 | 1985 | rVB6 | 1534   | 2372    | 0.12%  | 0.017% |
| 40 | 7.793  | 1999 | 2007 | 2015 | rBV7 | 2534   | 4682    | 0.24%  | 0.033% |
| 41 | 7.896  | 2025 | 2039 | 2055 | rBV  | 805111 | 1383384 | 71.78% | 9.814% |
| 42 | 8.179  | 2111 | 2127 | 2148 | rBV  | 167076 | 281857  | 14.62% | 2.000% |
| 43 | 8.401  | 2194 | 2196 | 2203 | rVB4 | 969    | 815     | 0.04%  | 0.006% |
| 44 | 8.459  | 2211 | 2214 | 2217 | rBV3 | 413    | 327     | 0.02%  | 0.002% |
| 45 | 8.555  | 2238 | 2244 | 2252 | rVB6 | 1229   | 1915    | 0.10%  | 0.014% |
| 46 | 8.633  | 2255 | 2268 | 2303 | rBV3 | 582366 | 1195513 | 62.03% | 8.481% |
| 47 | 8.915  | 2352 | 2356 | 2360 | rBV5 | 813    | 859     | 0.04%  | 0.006% |
| 48 | 8.964  | 2369 | 2371 | 2373 | rBV  | 402    | 259     | 0.01%  | 0.002% |
| 49 | 9.009  | 2382 | 2385 | 2390 | rVB2 | 443    | 299     | 0.02%  | 0.002% |
| 50 | 9.047  | 2390 | 2397 | 2400 | rBV3 | 657    | 588     | 0.03%  | 0.004% |
| 51 | 9.417  | 2499 | 2512 | 2533 | rBV  | 707278 | 1186623 | 61.57% | 8.418% |
| 52 | 9.571  | 2554 | 2560 | 2569 | rVB4 | 2182   | 3559    | 0.18%  | 0.025% |
| 53 | 9.694  | 2590 | 2598 | 2607 | rVB5 | 1840   | 2951    | 0.15%  | 0.021% |
| 54 | 9.835  | 2637 | 2642 | 2645 | rBV2 | 313    | 282     | 0.01%  | 0.002% |
| 55 | 9.954  | 2675 | 2679 | 2682 | rBV2 | 279    | 259     | 0.01%  | 0.002% |
| 56 | 10.009 | 2692 | 2696 | 2699 | rBV2 | 323    | 260     | 0.01%  | 0.002% |
| 57 | 10.102 | 2720 | 2725 | 2726 | rBV3 | 1100   | 892     | 0.05%  | 0.006% |
| 58 | 10.189 | 2749 | 2752 | 2758 | rVB2 | 224    | 244     | 0.01%  | 0.002% |
| 59 | 10.481 | 2838 | 2843 | 2845 | rBV2 | 1218   | 1079    | 0.06%  | 0.008% |
| 60 | 10.639 | 2884 | 2892 | 2896 | rBV4 | 3709   | 5421    | 0.28%  | 0.038% |
| 61 | 10.755 | 2915 | 2928 | 2948 | rBV  | 665950 | 1072948 | 55.67% | 7.612% |
| 62 | 10.867 | 2959 | 2963 | 2968 | rBV5 | 841    | 656     | 0.03%  | 0.005% |
| 63 | 11.021 | 3005 | 3011 | 3016 | rBV  | 294    | 357     | 0.02%  | 0.003% |
| 64 | 11.050 | 3016 | 3020 | 3026 | rBV2 | 415    | 465     | 0.02%  | 0.003% |
| 65 | 11.089 | 3026 | 3032 | 3041 | rVB5 | 972    | 1631    | 0.08%  | 0.012% |
| 66 | 11.160 | 3050 | 3054 | 3056 | rBV  | 303    | 242     | 0.01%  | 0.002% |
| 67 | 11.292 | 3091 | 3095 | 3096 | rBV  | 520    | 319     | 0.02%  | 0.002% |
| 68 | 11.388 | 3122 | 3125 | 3129 | rBV  | 302    | 279     | 0.01%  | 0.002% |
| 69 | 11.468 | 3144 | 3150 | 3156 | rVB6 | 2528   | 3251    | 0.17%  | 0.023% |
| 70 | 11.632 | 3198 | 3201 | 3205 | rVB2 | 384    | 259     | 0.01%  | 0.002% |
| 71 | 11.693 | 3215 | 3220 | 3224 | rVB3 | 878    | 721     | 0.04%  | 0.005% |
| 72 | 11.748 | 3229 | 3237 | 3244 | rVB5 | 3071   | 4349    | 0.23%  | 0.031% |
| 73 | 11.809 | 3244 | 3256 | 3279 | rBV  | 593423 | 954355  | 49.52% | 6.770% |
| 74 | 11.938 | 3294 | 3296 | 3302 | rVB3 | 1266   | 974     | 0.05%  | 0.007% |
| 75 | 11.973 | 3305 | 3307 | 3315 | rVB4 | 1775   | 1490    | 0.08%  | 0.011% |
| 76 | 12.015 | 3315 | 3320 | 3322 | rBV3 | 674    | 567     | 0.03%  | 0.004% |

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 12.192 | 3360 | 3375 | 3399 | rBV  | 739375 | 1194617 | 61.98% | 8.475% |
| 78  | 12.623 | 3505 | 3509 | 3512 | rBV2 | 585    | 409     | 0.02%  | 0.003% |
| 79  | 12.867 | 3581 | 3585 | 3588 | rBV2 | 468    | 318     | 0.02%  | 0.002% |
| 80  | 12.886 | 3588 | 3591 | 3595 | rBV3 | 348    | 273     | 0.01%  | 0.002% |
| 81  | 13.115 | 3659 | 3662 | 3665 | rBV2 | 338    | 270     | 0.01%  | 0.002% |
| 82  | 13.163 | 3672 | 3677 | 3681 | rVB  | 574    | 486     | 0.03%  | 0.003% |
| 83  | 13.224 | 3688 | 3696 | 3703 | rVV5 | 3346   | 5009    | 0.26%  | 0.036% |
| 84  | 13.275 | 3709 | 3712 | 3717 | rVB4 | 612    | 523     | 0.03%  | 0.004% |
| 85  | 13.410 | 3751 | 3754 | 3757 | rBV2 | 556    | 333     | 0.02%  | 0.002% |
| 86  | 13.504 | 3780 | 3783 | 3784 | rBV  | 420    | 250     | 0.01%  | 0.002% |
| 87  | 13.639 | 3821 | 3825 | 3827 | rBV2 | 526    | 432     | 0.02%  | 0.003% |
| 88  | 13.761 | 3860 | 3863 | 3869 | rBV4 | 499    | 440     | 0.02%  | 0.003% |
| 89  | 13.845 | 3880 | 3889 | 3897 | rBV5 | 5719   | 8898    | 0.46%  | 0.063% |
| 90  | 14.031 | 3945 | 3947 | 3953 | rBV2 | 368    | 257     | 0.01%  | 0.002% |
| 91  | 14.092 | 3958 | 3966 | 3979 | rVV2 | 7771   | 13051   | 0.68%  | 0.093% |
| 92  | 14.144 | 3979 | 3982 | 3986 | rVB2 | 701    | 486     | 0.03%  | 0.003% |
| 93  | 14.205 | 3998 | 4001 | 4005 | rBV  | 459    | 328     | 0.02%  | 0.002% |
| 94  | 14.330 | 4033 | 4040 | 4042 | rBV6 | 4373   | 4879    | 0.25%  | 0.035% |
| 95  | 14.980 | 4239 | 4242 | 4245 | rBV3 | 468    | 280     | 0.01%  | 0.002% |
| 96  | 15.140 | 4289 | 4292 | 4294 | rBV2 | 596    | 391     | 0.02%  | 0.003% |
| 97  | 15.201 | 4308 | 4311 | 4314 | rBV3 | 726    | 589     | 0.03%  | 0.004% |
| 98  | 15.362 | 4357 | 4361 | 4363 | rBV2 | 608    | 515     | 0.03%  | 0.004% |
| 99  | 15.410 | 4373 | 4376 | 4378 | rBV2 | 1043   | 685     | 0.04%  | 0.005% |
| 100 | 15.819 | 4499 | 4503 | 4509 | rBV7 | 1584   | 1764    | 0.09%  | 0.013% |

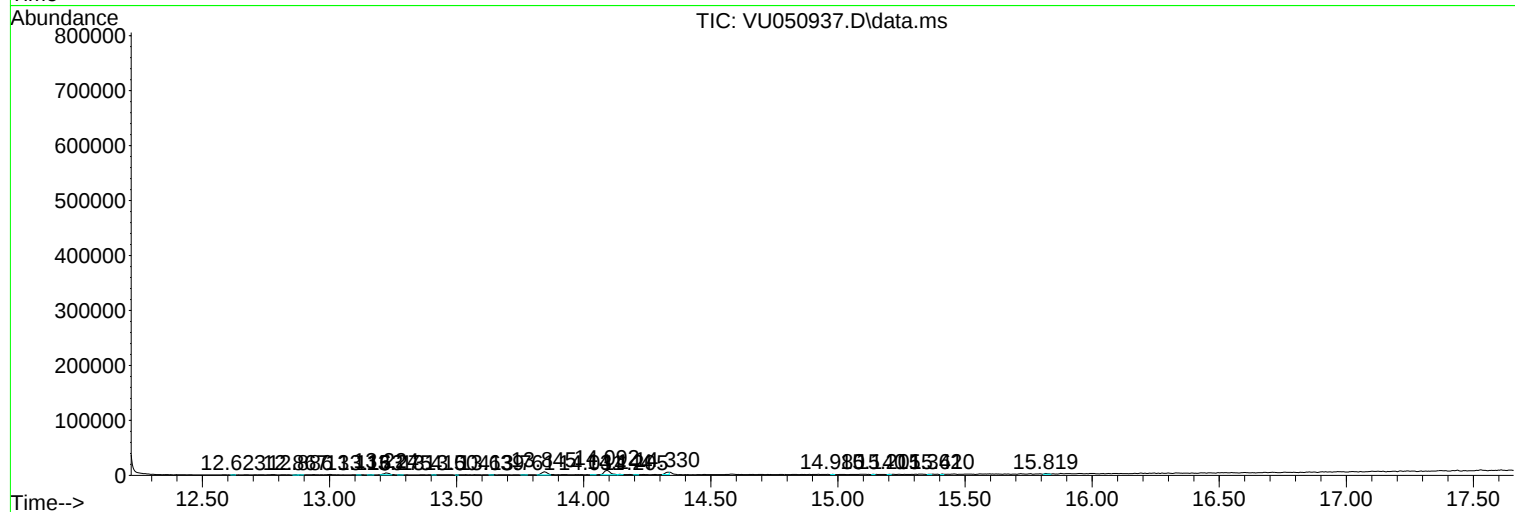
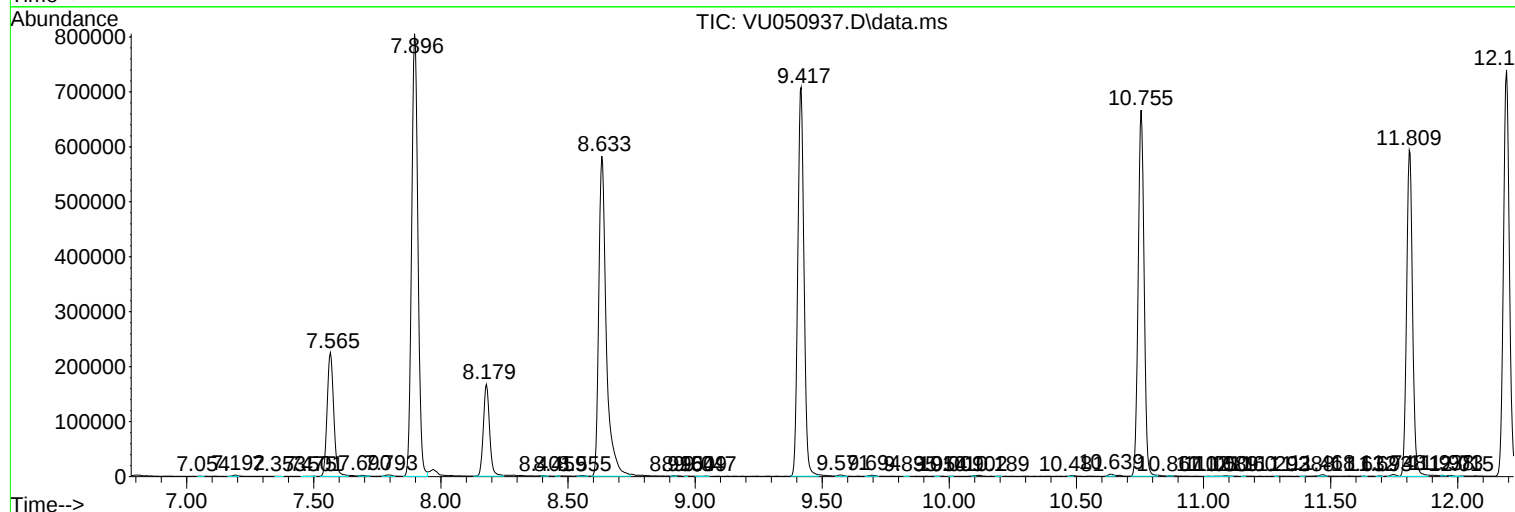
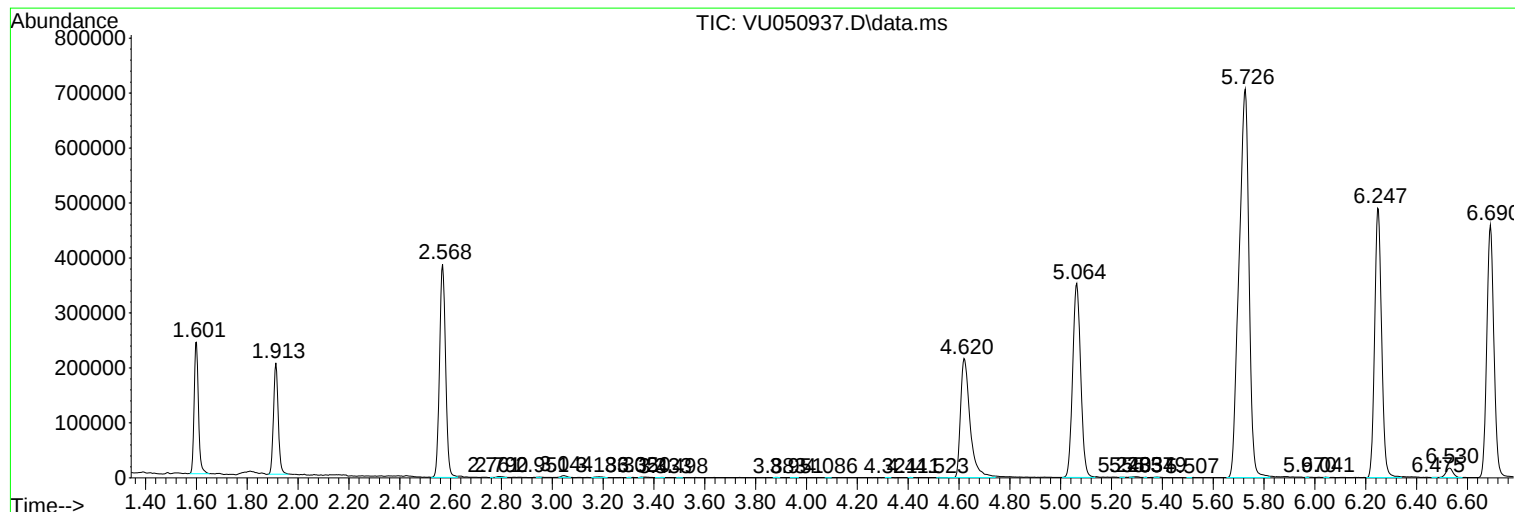
Sum of corrected areas: 14096247

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092022WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU092622\  
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No Library Search Compounds Detected

\*\*\*\*\*

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| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
|------------------|----|---------|-------|----------|---|----|------|------|
|------------------|----|---------|-------|----------|---|----|------|------|